COMPUTATIONAL FLUID DYNAMICS OF ADVANCED GAS DISPERSION: DEEP HOLLOW BLADE TURBINE

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ABSTRACT

Stirred tanks are widely used in the chemical and biochemical process industries. Mixing, fermentation, polymerization, crystallization and liquid-liquid extractions are significant examples of industrial operations usually carried out in tanks agitated by one or more impellers. The flow phenomena inside the tank are of great importance in the design, scale-up and optimization of tasks performed by stirred tanks. This work presents of a stirred tank agitated by an advanced gas dispersion impeller namely deep hollow blade turbine (HEDT) using Computational Fluid Dynamic (CFD) method. The standard k-ε, realizable k-ε and shear-stress transport k-ϖ were considered in this study for comparison purposes. Predictions of the impeller-angle-resolved and time-averaged turbulent flow have been evaluated and compared with data from Particle Image Velocimetry (PIV) measurements. Multiple Reference Frame (MRF) used to capture flow features in details and predicts flow for steady state for the impeller blades relative to the tank baffles. Unsteady solver indeed predicts periodic shedding, and leads to much better concurrence with available experimental data than has been achieve with steady computation.

ABSTRAK

Tangki pengacau digunakan secara meluas dalam industri pemprosesan kimia dan biokimia. Proses pengacauan, penapaian, pempolimeran, penghabluran dan pengekstrakan cecair adalah contoh ketara operasi di dalam industri yang biasanya dilakukan di dalam tangki pengacau menggunakan satu *impeller* atau lebih. Fenomena aliran di dalam tangki amat penting dalam proses mereka bentuk, meningkatkan skala dan optimumkan prestasi tanki pengacau. Kajian ini membentangkan tangki pengacau menggunakan *impeller* terkini untuk sebaran gas yang maju iaitu *deep hollow blade turbine* (HEDT) menggunakan kaedah *Computational Fluid Dynamic* (CFD). *Standard k-ε*, *realizable k-ε* dan *shear-stress transport k-ω* dipertimbangkan untuk tujuan perbandingan kajian ini. Ramalan *impeller-angle resolve* dan aliran *turbulent* berdasarkan masa telah dinilai dan dibandingkan dengan data yang diukur menggunakan kaedah *Particle Image Velocimetry* (PIV). *Multiple Reference Frame* (MRF) digunakan untuk mengetahui ciri-ciri aliran dengan terperinci dan meramalkan aliran untuk *steady state* untuk *impellers* dan *baffles* di dalam tangki. *Unsteady solver* digunakan untuk meramalkan penumpahan berkala dan membawa kepada data yang lebih bertepatan dengan data eksperimen yang dicapai menggunakan *steady solver*.

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LIST OF SYMBOLS

σ_k	-	Constant for eq.(3-1)
σ_ε	-	Constant for eq. (3-2)
$C_{1\varepsilon}$	-	Constant for eq. (3-5)
β_{i1}	-	Constant for eq. (3-14)
β_{i2}	-	Constant for eq. (3-14)
$C_{2\varepsilon}$	-	Constant for eq. (3-5)
C_μ	-	Constant for eq. (3-3)
D	-	Impeller diameter, m
ε	-	Turbulent energy dissipation rate
H	-	Liquid height in the tank, m
k	-	Turbulent kinetic energy, $m^2.s^{-1}$
N	-	Rotational speed, s^{-1}
Re	-	Reynolds number
T	-	Tank diameter, m
$Utip$	-	Impeller tip velocity, $m.^{s-1}$

LIST OF ABBREVIATIONS

SM	-	Sliding mesh
MRF	-	Multiple Reference Frames
CFD	-	Computational Fluid Dynamics
LES	-	Large-eddy Simulation
RANS	-	Reynolds-averaged Navier-Stokes
et al.	-	and others
LDA	-	Laser Doppler Anemometer
PIV	-	Particle Image Velocity
SKE	-	Standard k-ε
RKE	-	Realizable k-ε
SST k-ϖ	-	Shear-stress-transport k-ϖ
HEDT	-	Deep hollow blade (semi-ellipse) disc turbine
RT	-	Rushton turbine

CHAPTER 1

INTRODUCTION

1.1 MOTIVATION

Stirred tank is widely used in chemical, mineral and biochemical industries and waste water treatment. In the majority cases, the flow field in baffled stirred tank is highly turbulent hence it is three-dimensional and complex in nature. There have been continuous efforts on understanding these flows using whether experimental or computational dynamics tools.

Understanding the model and design fluid flow whether single phase or multiple phases would allow for better performance and decrease waste due to inadequate design. More than 15 years ago, it is estimated that nearly half of the $750 billion annual output from chemical industry alone passed through a stirred tank at one point and that losses incurred by inadequate design were on the order of tens of billions of dollars (Tatterson et al., 1991) and about 50% of all chemical productions take place in stirred tank (Butcher and Eagles, 2002). Therefore, adequate design with lower cost can be simulated by using Computational Fluid Dynamics (CFD) to achieved advanced gas dispersion using deep hollow blade turbine.

1.2 PROBLEM STATEMENT

Gas dispersion technology is important. The design must consider the flow filled in baffled stirred tank and turbulent kinetics energy.

For several decades, the Rushton turbine was the standard impeller for gas dispersion applications. It features six flat blades mounted on a disk. The flat blade of the Rushton turbine leads to the formation of a pair of high-speed, low-pressure trailing vortices at the rear of each blade. Those vortices provide the source of turbulence and are identified as the major flow mechanism responsible for mixing and dispersion in stirred tanks. However, the trailing vortices lead to a high power number under ungassed conditions which gives rise to a high torque for a given rotating speed and hence a high operating cost.

Then, John M. Smith and coworkers introduced the concept of using concave blades. They explained the improved performance of the concave blades compared to flat blades in terms of reduced cavity formation behind the blades (Bakker et al., 2000). Hence, the attached gas bubble does not affect the drag in the same way as it does with a flat blade. So the power loss is much less compared with the flat blade. Latterly, impellers with a semi-circular blade shape are introduced for example CD-6 (symmetric blade) and BT-6 (asymmetric blade).

Relatively recent, new blade impeller has been introduced. Deep hollow blade turbine (HEDT) is more effective for gas-liquid dispersion and liquid-liquid dispersion even though it can be used for any type of single-phase and multiple phase mixing duty. As radial flow impellers, it will discharge fluid radially outward to the vessel wall while with suitable baffles these flows are converted to strong top-to-bottom flows above and below the impeller. Therefore, the elliptical shape reduces the cavity size, great reduction of the trailing vortex and results in much less power drop when gassed. HEDT would handle high gas rates without significant loss of power under fully loaded conditions. Therefore, studies on the HEDT are helpful for better gas dispersion in mechanically stirred tank.

Experimental for investigating the structure and behavior of gas dispersion have been done previously using advanced methods such as time-resolved particle image velocimetry (TRPIV) and Laser-Droppler Anemometry (LDA) (Gao et al., 2010). LDA to measure the angle resolved is essentially a single point technique. Therefore, instantaneous measurements of large-scale structures are not possible with LDA. PIV is a whole field technique to characterize instantaneous flow structures around rotating impeller blades. Yet, these methods have limitations according to their affordability as both are expensive, difficulties in set-up and harmful based on the laser used. Thus, computational fluid dynamics (CFD) is an increasingly important tool for carrying out realistic simulations of process equipment (Scargiali et al., 2007). CFD can be used as a design tool or as a design guide to compare the performance of HEDT in stirred tank with decreasing cost to evaluate without undertaking expensive experimental pilot or laboratory to test of all parameters required.

1.3 OBJECTIVE AND SCOPE

The aim of this study is to develop a modeling method for hydrodynamics. In this paper, the flow fields and turbulence kinetics energy in stirred tank with deep hollow blade turbine were investigated by using a computational fluid dynamics (CFD). The CFD model used to validate the flow patterns and gas dispersion performance using HEDT by comparing the results with publish results. The first scope of this research is to predict velocity profile and turbulence kinetics energy (TKE) of stirred tank agitated with HEDT. The second part is to predict the effect of discretisation method and grid analysis.

1.4 SIGNIFICANT OF STUDY

Maximizing profits by operating the most efficient process is the primary goal of all industrial operations such as fermentation, pharmaceutical and biochemical. Process simulation which is the application of a range of software tools to analyze complete processes creates efficient operation at inexpensive workstations. In addition, many qualitative features of the flow field can be difficult to be determined experimentally. Process engineers and scientists use simulation models to investigate complex and integrated biochemical operations without the need for extensive experimentation (Gosling, 2005). A recent development in modeling is the use of Computational Fluid Dynamics (CFD). Model developed in this work via CFD is useful tool to investigate single and multiphase stirred tank operations without the need for extensive experimental setup as prototype and pilot scale testing can be time-consuming and expensive. Therefore, studying the fluid dynamics of advanced gas dispersion using deep hollow blade turbine (HEDT) enable to predict and understand the process flow condition while reducing costs and time-to-market.

1.5 MAIN CONTRIBUTION OF THIS WORK

Deep hollow blade turbine (HEDT) is an effective impeller for gas-liquid dispersion and liquid-liquid dispersion for any type of single-phase or multiple phases mixing. Most of the researchers done in mixing area are limited to experimental method to examine the flow structures developed in stirred vessel such as Laser-Doppler Anemometry (LDA) and Particle Image Velocity (PIV) method. Recent publications have established the potential of computational fluid dynamics (CFD) using Rushton impeller which has been recognized for several decades followed by concave blades and impellers with a semi-circular blade shape for example CD-6 (symmetric blade) and BT-6 (asymmetric blade). Therefore, in this work it is necessary to investigate the ability of HEDT as until now, no research available which evaluate turbulence models or flow distributions for mechanical agitation using HEDT by CFD method as this method has now become a powerful tool for prediction of fluid flows and mixing time in stirred vessels.

1.6 STRUCTURE OF THIS WORK

The structure of the thesis is outlined as follow:

Chapter 2, the literature review provides general description on the flow characteristics provided with a brief discussion from the previous work related to advanced experimental techniques available. The applications and limitation of method also stated.

Chapter 3, the CFD approach presenting the turbulence modeling, velocity characteristics and solution procedures.

Chapter 4, the results for effect of discretisation method, grid dependent analysis, effect of turbulence model and comparison between steady and unsteady simulation were compared with predicted results from experimental data. This chapter validates the experimental published data by Gao et al. (2010) with the CFD model.

Chapter 5, the conclusions of this study and recommendations for future work are given.

CHAPTER 2

LITERATURE REVIEW

2.1 OVERVIEW

This chapter will be covered on the description of deep hollow blade turbine (HEDT) that shows the suitability to achieved better gas dispersion. Experimental and simulation work has been reported in the published literature. Hence, the present work reviews on the computational work on the velocity and turbulent kinetics energy

2.2 INTRODUCTION

An impeller that approximately maintains the ungassed power level when gas is introduced will give more stable operation and minimal scale-up difficulties. Deep hollow blade turbine suitable for advance gas dispersion as it will control the flooding point, loaded condition and hold up. Then, flooding point is the point where the gas bubbles are not driven to the tank wall roughly within the plane of the impeller. Therefore, this impeller can avoid flooding which a condition that more gas is entering than it is effectively able to disperse with radial agitators to achieved complete dispersion whereby the gas bubbles are distributed throughout the vessel and significant gas is circulated back to the impeller.

Although they can be used for any type of single-phase and multiple phase mixing duty, they are most effective for gas-liquid dispersion. Radial flow impeller discharge fluid radially outward to the vessel wall while with suitable baffles, this flow is converted to strong top-to-bottom flows both above and below the impeller. Under fully loaded conditions in which the impeller disperses the gas through the upper part of the vessel, the hollow blade turbine will handle high gas rate without significant loss of power. This is a function of the degree of streamlining as the design of blade ensures it achieves the minimum Froude number (Cooke et al., 2005). Froude number is to correlate power draw in gas-liquid systems where gravity has a significant influence due to the low density of gas bubbles and their strong tendency to rise.

Based on the idea that gas rises, the gas pocket or cavities must be eliminated so as to minimize power drop on the low pressure side and high gas flow rates of the blade. So that, deep hollow blade shape reduces the cavity size and provide better gas dispersion as the gas is being dispersed from inside of the blade, reduces streamlining, much less power drop when gassed and increases net pumping. Therefore, it also improves holding up capacity.

2. 3 APPLICATION OF STIRRED TANK DISPERSION

2.3.1 Bioreactor Fermentation

One common goal in plant cell bioreactor design is to develop a reactor that provides a prolonged, sterile, culture environment with efficient mixing and oxygen transfer without producing excessive foaming and hydrodynamics shear at low cost. Down-pumping mode in viscous *Streptomyces* fermentation gave better oxygen transfer with very little power drops of gassing even at very high impeller flow rates. Therefore, deep hollow blade turbine is expected to be well suited for dispersing gas in bioreactors where a wide range of gas is required (Yang et al., 2007).

2.3.2 Reactive Crystallization

Reactive crystallization presents critical mixing issues because mixing affects both the reaction and crystallization step. Those difficulty with reactive crystallization scale-up due to the need to balance the requirements to achieve a growth-dominated process, choose a mixing system fast enough to micro-mix effectively for the fast reaction and ensure mixing is not too powerful that it will cause crystal fracture. Macro mixing performance for the optimization of the configurations and operating conditions provided with fully turbulent flow. Apart from macro mixing performance, micro mixing performance indicators such as turbulent kinetic energy and local energy dissipation rate are also important in processes, especially for crystallization (Li et al., 2005).

2.4 EXPERIMENTAL METHOD OF STIRRED TANK DISPERSION

There are several technique used to study on the gas dispersion which consists of Laser-Doppler Anemometry (LDA) and Time-Resolved Particle Image Velocimetry (TRPIV) instead of Computational Fluid Dynamics (CFD) method.

2.4.1 Laser-Doppler Anemometry (LDA)

Laser-Doppler Anemometry (LDA) is a technology to measure velocities of gasses at a point in a flow using light beams from a laser especially for small particles in flows. This technique senses true velocity and measures the laser light scattered by particles that pass through a series of interference fringes (a pattern of light and dark surfaces). A laser beam is split into two beams with one propagated out of the anemometer. Scattered light from particles passing through is focused and send the light back into a detector to measure relative to the original laser beam. A beat frequency corresponding to the difference in Doppler shifts from the two scattered beams is obtained since the light scattered from both beams reaches the detector simultaneously. Therefore, the beat frequency is directly proportional to the velocity component perpendicular to the fringe geometry which emerges in the cross section.

2.4.2 Time-Resolved Particle Image Velocimetry (TRPIV)

Time-Resolved Particle Image Velocimetry (TRPIV) consists of a laser with sheet optics, one or two digital cameras and a computer with a timer unit to control the system and storing data. The movement of a group of particles flows can be determined as two consecutive short-duration light pulses produced by a laser scattered from the particles is acquired during both laser pulse by a digital camera and stored for analysis. Displacement of the particles between the laser pulses gives estimation of velocity of the particles. As it able to do time-resolve PIV, several thousand velocity fields per second can be obtained.

2.5 STUDIES ON STIRRED TANK DISPERSION

In previous, experimental and CFD studies have been conducted by many researchers. These studies provide valuable information on hydrodynamics in stirred tank using different type of impellers and turbulent model. Some of the work is summarized in Table 2.1. The majority of the results include data which can be used for the validation of further CFD investigation and the optimum design of the blade impeller in stirred tank. Therefore, the aim of this work is to improve the CFD prediction for HEDT impeller in stirred tank.

Table 2.1 Study of deep hollow blade turbine

Authors	**System investigated**	**Turbulence Model**	**Remarks**
Alcamo et al. (2005)	Rushton impeller, unbaffled vessel D = 0.19m, $H = T$, N = 200rpm, $Re = 3 \times 10^4$	Large eddy simulation (LES)	An excellent agreement between experimental data (PIV) for unbaffled vessel and CFD simulation using LES especially regarding mean tangential velocities. Good agreement was also observed for radial average velocities.
Aubin et al. (2004)	Pitched blade turbine, (simulations are validated using experimental LDV results obtained by the same group of authors)	k-ε model, RNG model	The CFD simulations have been validated by laser doppler velocimetry (LDV). A first order method underestimate LDV data compared to higher order methods. The type of the turbulence model was limited to the k-ε and RNG models due to convergence difficulties encountered with a Reynolds stress model. Little effect on the mean flow and turbulent kinetic energy were found by using those turbulence models.
Gao et al. (2008)	RT6, CD6, HEDT impellers, T = 0.48m, T/10, D = 0.034m, H = 0.25m, electrical input = 3, 6,9 and12kW	no	The study proves that HEDT impeller operates well in a boiling suspension, maintaining suspension at lower specific power input rather than BT6 and CD6 impellers.
Gao et al. (2010)	HEDT impeller, T = 0.19m, D = 0.4T, $H = T$, N = 90rmin^{-1}, Re = 8847	no	This study compared experimental values of radial velocity, axial velocity, vorticity, the random turbulent kinetic energy and periodic kinetic energy obtained from traditional PIV and TRPIV. The evaluation of the impeller stream was observed clearly from both methods.

Table 2.1 Study of deep hollow blade turbine (Continued)

Authors	System investigated	Turbulence Model	Remarks
Gao et al. (2011)	RT, CD, HEDT and PDT impellers, D = 0.48m	no	PIV technique used to study the trailing vortices and the distribution of turbulent kinetic energy. Disc turbine shape of blade decreases the power input. The phase-averaged turbulent kinetic energy show the turbulent kinetic energy becomes smaller as the blade turns more curved. As the blade turns more curved, the inclination of the impeller stream become smaller and the radial jet becomes weaker.
Hartmann et al. (2004)	Sliding mesh (SM), Rushton turbine, T = 150mm, H = T, N = 2627 rpm	Large eddy simulations (LES), Reynolds-averaged Navier-Stokes (RANS) – shear-stress transport (SST) model	A transient RANS simulation is able to provide an accurate representation of flow field but fails in the prediction of the turbulent kinetic energy compared to the LES model.
Jahoda et al. (2009)	Sliding mesh (SM) method, Multiple Reference Frames (MRF) method, PBT impeller, T = 0.29m, T/10, H=T, N = 300 rpm, Re = 4.66×10^4	Standard k-ε Eulerian-Eulerian approach	CFD simulation of a gas-liquid two-phase flow predicted using RANS technique. The results show a good agreement with experiment based on prediction of liquid homogenization using SM method while MRF method is sufficient mainly for higher volumetric gas flow rate.

Table 2.1 Study of deep hollow blade turbine (Continued)

Authors	System investigated	Turbulence Model	Remarks
Jaworski and Zakrzewska (2002)	Pitched blade turbine, T = 0.202m, H = T, N = 290 rpm, Re = 22,500	Standard k-ε, RNG k-ε model, realizable k-ε model, Chen-Kim k-ε, optimized Chen-Kim k-ε, Reynolds stress model	Simulation results were compared with LDA experimental data. The axial velocity component was predicted well by using standard k-ε model and the optimized Chen-Kim k-ε model while turbulent kinetic energy was significantly underpredicted for all models. However, standard k-ε delivered the smallest deviations from experiment.
Khopkar et al. (2006)	Pitched blade turbine, T = 0.3m, H = 0.9m, T/10, N = 100, 145 and 390 rpm, d_s = 0.1mm	Standard k-ε	CFD model used to investigate the turbulent gas-liquid flows generated by three down-pumping pitched blade turbines. Flow field generated by three-down pumping pitched blade turbine, including the liquid circulation loops and the dispersion quality of gas is captured.
Kshatriya et al. (2007)	Multiple Reference Frame (MRF) method, BT6, ICI gasfoil, PBIUP and PBIDIN impeller, N = 10rps, superficial gas flow = 0.130 m/s, D = 0.57m,	k-ω model	CFD is shown as a useful tool to predict the experiment on cavity formation on impeller and gas dispersion pattern (gas holdup and transition regimes). Larger the cavity, larger the power drop. Based on experimental observation and CFD performance, PBIUP gives a better gas performance. PBIUP is modified impeller which made asymmetric with the extension of upper part.

Table 2.1 Study of deep hollow blade turbine (Continued)

Authors	**System investigated**	**Turbulence Model**	**Remarks**
Murthy and Joshi (2008)	DT, PBT (60,45 and 30) and HF impeller, $H = T$, $T/10$, T = 0.30m,	Standard k-ϵ Reynolds stress model (RSM) Large eddy simulation (LES)	Mean flow field and turbulent kinetic energy measured using LDA was compared with CFD simulations performed by Standard k-ϵ, Reynolds stress model (RSM) and Large eddy simulation (LES). For mean flow predictions, RSM performed better than the standard k-ϵ as standard k-ϵ performs well when the flow is unidirectional that is with less swirl and weak recirculation. Both Standard k-ϵ and RSM fail to predict the turbulent kinetics energy in the impeller region when the flow is dominated by the unsteady coherent flow structures. However, LES has strength of the precessing vortex instability and turbulent kinetics energy. So DT has identified produces strongest instabilities while HF generates the weakest instabilities.
Myer et al. (1999)	BT-6, PD-6, D-6 and CD-6 impellers, D = 0.44m, 0.60m and 1.52m, $T/12$, superficial gas velocity = 0.007-0.07ms^{-1}, power input = 400-4000Wm^{-3}, Re = 10-2000000	no	From experiment data, performance of gas dispersion can be significantly improved by using deep blades that are vertically asymmetric. It has a gassed number which lower than other impellers. It also can disperse more gas before flooding and no gas filled cavities were observed from the inside of the blade.